

Generalization of the Brodsky-Lepage-Mackenzie optimization within the $\{\beta\}$ -expansion and the Principle of Maximal Conformality

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Abstract

We discuss generalizations of the BLM optimization procedure for renormalization group invariant quantities. In this respect, we discuss in detail the features and construction of the $\{\beta\}$ -expansion representation instead of the standard perturbative series with regards to the Adler D -function and Bjorken polarized sum rules obtained in order of $\mathcal{O}(\alpha_s^4)$. Based on the $\{\beta\}$ -expansion we analyse different schemes of optimization, including the corrected Principle of Maximal Conformality, numerically illustrating their results. We suggest our scheme for the series optimization and apply it to both the above quantities.

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1. INTRODUCTION

The problem of scale-scheme dependence ambiguities in the renormalization group (RG) calculations [1] remains important. In the past few years, a new extension of the BLM scale-fixing approach [2], called the Principle of Maximal Conformality (PMC), was started [3] and formulated in more detail in [4–7] with a variety of applications to phenomenologically oriented studies.

Here we show that the PMC approach is closely related to the sequential BLM (seBLM) method, originally proposed in [8] for the analysis of the N²LO QCD prediction for the quantities like e^+e^- -annihilation R-ratio. This method was based on the renormalization group (RG) inspired representation of the $\{\beta\}$ -expansion for perturbative series, the one later used for other purposes in [9, 10]. The seBLM was constructed as a generalization of the works devoted to the extension of the BLM $\overline{\text{MS}}$ -type scale fixing prescription to the level of next-to-next-to-leading order (N²LO) QCD corrections [11, 12] and beyond [13–16].

In this paper, we will use the $\{\beta\}$ -expansion representation and the seBLM method to study the e^+e^- -annihilation R-ratio, the related Adler function D^{EM} of the electromagnetic quark currents and the Bjorken sum rule S^{Bjp} of the polarized lepton-nucleon deep-inelastic scattering (DIS). We will clarify the concrete theoretical shortcomings of the PMC QCD studies performed in a number of works on the subject, in particular, in Refs. [4–7], and will present the results for the corrected PMC approach.

Certain problems of the misuse of the PMC approach to the Adler function were already emphasized in [17] but not recognized in the recently published work [7]. We will clarify these theoretical problems in more detail and consider the existing modification of the N²LO PMC analysis, based on application of the seBLM method, which allows one to reproduce the original NLO BLM expression from the considerations performed in [7] and already discussed in [17]. Note that the necessity of introducing modifications to the analysis of [7] starts to manifest itself from the level of taking into account the second order perturbative corrections to the R-ratio evaluated analytically in [18] in the minimal subtractions (MS) scheme proposed in [19]. This result was also obtained numerically in [20] and confirmed analytically in [21] by using the $\overline{\text{MS}}$ -scheme of [22]. At the level of the third order corrections to D^{EM} , analytically calculated in the $\overline{\text{MS}}$ scheme [23, 24] and confirmed in the independent work [25], there appear additional differences between the results of the PMC and the seBLM methods.

We present several arguments in favour of theoretical and phenomenological applications of the form of the β -expanded expressions for the RG invariant (RGI) quantities proposed in [8] and applied in [9]¹. In this respect, let us mention the QCD generalization (in $\overline{\text{MS}}$ -scheme) of the Crewther relation [27] based on the $\{\beta\}$ -expansion [9]. Using the results of these relations we obtain in a self-consistent way the N²LO $\{\beta\}$ -expansion for $S^{\text{Bjp}}(Q^2)$ in QCD with $n_{\tilde{g}}$ -numbers of gluinos, which can be checked by direct analytical calculations.

The article is organized as follows. In Sec. 2, we define single-scale RG invariant quantities for the e^+e^- -annihilation to hadrons and for the DIS inclusive processes, which will be studied in this work. The existing theoretical relations between perturbative expressions for these characteristics are also summarized. In Sec. 3, the $\{\beta\}$ -expansion of the RGI

¹ Note, that the $\{\beta\}$ -expansion representation is related in part to the considered in [26] expansion of the perturbative terms in the RG invariant (RGI) Green functions through the powers of the first coefficient of the β -function

quantities, proposed in [8] and applied in [9, 10], is reminded and discussed in detail. Using the results of [8] and the “multiple power β -function” QCD expression [9] for the $\overline{\text{MS}}$ -scheme generalization of the Crewther relation [27] we provide the arguments that this expansion is unique. The details of constructing the $\{\beta\}$ -expansions for the Adler D^{EM} function and for the S^{Bjp} sum rule are described at the level of the $O(a_s^3)$ -corrections, where $a_s = \alpha_s/(4\pi)$. In Sec. 4.1, we consider the relations between certain terms of the $\{\beta\}$ -expansion for D^{EM} and S^{Bjp} , which will be obtained from the Crewther relation of [27] and its QCD generalization of [9], and present the concrete $\{\beta\}$ -expanded contributions to the D^{EM} function, R-ratio and the S^{Bjp} sum rule.

Using our definition of the $\{\beta\}$ -expansion representation we correct the values of the PMC coefficients and the scales in the related powers of the PMC perturbative expressions for the Adler function D^{EM} and $R_{e^+e^-}$ -ratio, presented in [4–7], and discuss their correspondence to the results obtained in [8, 9, 17]. The discussion of the results of the BLM, seBLM, PMC procedures together with the numerical estimates of the corresponding perturbation theory (PT) coefficients and the couplings at new normalization scales are presented in Sec. 5. It is demonstrated that in spite of its theoretical prominence following from the conformal symmetry relations even the corrected PMC procedure does not improve the convergence of perturbative series for the R -ratio and for the S^{Bjp} sum rule. The methods of further optimizations of these series, which are based on the $\{\beta\}$ -expansion, are elaborated in Sec. 6. The technical results are presented in the appendices.

2. DEFINITIONS OF THE BASIC QUANTITIES

Consider first the Adler function $D^{\text{EM}}(Q^2)$, which is expressed through the two-point correlator of the electromagnetic vector currents $j_\mu^{\text{EM}} = \sum_i q_i \bar{\psi}_i \gamma_\mu \psi_i$ taken at Euclidean $-q^2 = Q^2$. Here q_i stands for the electric charge of the quark field ψ_i . $D^{\text{EM}}(Q^2)$ consists of the sum of its nonsinglet (NS) and singlet (S) parts

$$D^{\text{EM}}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right) = \left(\sum_i q_i^2\right) d_R D^{\text{NS}}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right) + \left(\sum_i q_i\right)^2 d_R D^{\text{S}}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right), \quad (2.1a)$$

where

$$D^{\text{NS}}(Q^2/\mu^2, a_s(\mu^2)) = 1 + \sum_{l \geq 1} d_l^{\text{NS}}(Q^2/\mu^2) a_s^l(\mu^2), \quad (2.1b)$$

$$D^{\text{S}}(Q^2/\mu^2, a_s(\mu^2)) = \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} d_l^{\text{S}}(Q^2/\mu^2) a_s^l(\mu^2). \quad (2.1c)$$

Here d_R is the dimension of quark representation of $SU(N_c)$ color gauge group ($d_R = N_c$) and $d^{abc} = 2\text{Tr}\left(\left\{\frac{\lambda_a}{2}, \frac{\lambda_b}{2}\right\} \frac{\lambda_c}{2}\right)$ is the symmetric tensor. Both the NS and S contributions to the Adler-function are the RGI quantities calculable in the Euclidean domain. After applying the RG equation they can be represented as

$$D^{\text{NS}}(Q^2/\mu^2, a_s(\mu^2)) \xrightarrow{\mu^2=Q^2} D^{\text{NS}}(a_s(Q^2)) = 1 + \sum_{l \geq 1} d_l^{\text{NS}} a_s^l(Q^2) \quad (2.2a)$$

$$D^{\text{S}}(Q^2/\mu^2, a_s(\mu^2)) \xrightarrow{\mu^2=Q^2} D^{\text{S}}(a_s(Q^2)) = \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} d_l^{\text{S}} a_s^l(Q^2). \quad (2.2b)$$

Due to the cancellation of the logarithms $\ln^k(Q^2/\mu^2)$ with $k \geq l+1$ in the terms $d_i^a(Q^2/\mu^2)$ (the superscript a defines the contributions to the NS and S parts of the D^{EM} -function) the coefficients of $d_l^a \equiv d_l^a(1)$ are the numbers in the MS-like schemes.

Let us emphasize that in this work we use the perturbative expansion parameter $a_s(\mu^2)$ normalized as $a_s(\mu^2) \equiv \alpha_s(\mu^2)/4\pi$. It obeys the RG equation with the consistently normalized $SU(N_c)$ -group β -function

$$\mu^2 \frac{d}{d\mu^2} a_s(\mu) = \beta(a_s) = -a_s^2 \sum_{i \geq 0} \beta_i a_s^i, \quad (2.3)$$

where $\beta_0 = (11/3C_A - (4/3)T_R n_f)$ while other coefficients β_i are presented in Appendix A.

The quantity related to the observable total cross-section of the $e^+e^- \rightarrow \text{hadrons}$ process $R_{e^+e^-}(s) = \sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$ is measured in the Minkowski region ($s > 0$); this can be obtained from the D^{EM} -function as

$$\begin{aligned} R_{e^+e^-}(s) &\equiv R(s, \mu^2 = s) = \frac{1}{2\pi i} \int_{-s-i\varepsilon}^{-s+i\varepsilon} \frac{D^{\text{EM}}(\sigma/\mu^2; a_s(\mu^2))}{\sigma} d\sigma \Big|_{\mu^2=s} = \\ &= \left(\sum_i q_i^2 \right) d_R \left(1 + \sum_{m \geq 1} r_m^{\text{NS}} a_s^m(s) \right) + \left(\sum_i q_i \right)^2 \frac{d^{abc} d^{abc}}{d_R} \sum_{n \geq 3} r_n^{\text{S}} a_s^n(s) \end{aligned} \quad (2.4)$$

The coefficients r_m^a for the a part ($a = \text{NS}$ or S) of $R_{e^+e^-}$ are associated with the coefficients d_l^a of the D^a function by the triangular matrix T^a of the relation $r_m^a = T_{ml}^a d_l^a$, which will be discussed in subsection 4.3 and Appendix C.

The next observable RGI quantity, we will be interested in, is the Bjorken polarized sum rule S^{Bjp} . It is defined by the integral over the difference of the spin-dependent structure functions of the polarized lepton-proton and lepton-neutron deep-inelastic scattering as

$$S^{\text{Bjp}}(Q^2) = \int_0^1 [g_1^{lp}(x, Q^2) - g_1^{ln}(x, Q^2)] dx = \frac{g_A}{6} C^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)), \quad (2.5)$$

where g_A is the nucleon axial charge as measured in the neutron β -decay, and $C^{\text{Bjp}}(a_s)$ is coefficient function calculable within perturbation theory and not damped by the inverse powers of Q^2 , i.e., the leading twist term.

The application of the operator-product expansion (OPE) method in the MS-like scheme [28] and the knowledge on the perturbative structure of the $\overline{\text{MS}}$ -scheme QCD generalization of the quark-parton model Crewther relation [27] gained from articles in [29–35] indicate the existence of the previously undiscussed singlet contribution to $C^{\text{Bjp}}(a_s)$ [36]. Using the results of this work we define the overall perturbative expression for C^{Bjp} as

$$C^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) = C_{\text{NS}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) + \left(\sum_i q_i \right) C_{\text{S}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) \quad (2.6)$$

where the NS and S coefficient functions can be written down as

$$C_{\text{NS}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) = 1 + \sum_{l \geq 1} c_l^{\text{NS}}(Q^2/\mu^2) a_s^l(\mu^2) \quad (2.7)$$

$$C_{\text{S}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) = \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} c_l^{\text{S}}(Q^2/\mu^2) a_s^l(\mu^2), \quad (2.8)$$

and have the following RG-improved form

$$C_{\text{NS}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) \xrightarrow{\mu^2=Q^2} C_{\text{NS}}^{\text{Bjp}}(a_s(Q^2)) = 1 + \sum_{l \geq 1} c_l^{\text{NS}} a_s^l(Q^2), \quad (2.9a)$$

$$C_{\text{S}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) \xrightarrow{\mu^2=Q^2} C_{\text{S}}^{\text{Bjp}}(a_s(Q^2)) = \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} c_l^{\text{S}} a_s^{l+1}(Q^2), \quad (2.9b)$$

$$C^{\text{Bjp}}(a_s(Q^2)) = C_{\text{NS}}^{\text{Bjp}}(a_s(Q^2)) + C_{\text{S}}^{\text{Bjp}}(a_s(Q^2)). \quad (2.9c)$$

The analytical expressions for the NLO and N²LO corrections to Eq.(2.9a) in the $\overline{\text{MS}}$ -scheme were evaluated in [37] and [38], respectively, while the corresponding N³LO $\mathcal{O}(a_s^4)$ -correction was calculated in [33] (its direct analytical form was also presented in [9]). The symbolic expression for the coefficient c_4^{S} of the $\mathcal{O}(a_s^4)$ -correction to the singlet contribution $C_{\text{S}}^{\text{Bjp}}(a_s)$ of the Bjorken polarized sum rule was fixed in [36] from the $\overline{\text{MS}}$ -scheme generalization of the Crewther relation, which will be presented below.

Let us also consider the Gross-Llewellyn Smith (GLS) sum rule of the deep-inelastic neutrino-nucleon scattering. Its leading twist perturbative QCD expression can be defined as

$$S_{\text{GLS}}(Q^2) = \frac{1}{2} \int_0^1 [F_3^{\nu p}(x, Q^2) + F_3^{\nu n}(x, Q^2)] dx = 3C_{\text{GLS}}(Q^2/\mu^2, a_s(\mu^2)) \quad (2.10)$$

where $F_3(x, Q^2)$ is the structure functions of the deep-inelastic neutrino-nucleon scattering process. The coefficient function in the RHS of Eq.(2.10) also contains both NS and S contributions, namely

$$C_{\text{GLS}}(Q^2/\mu^2, a_s(\mu^2)) = C_{\text{GLS}}^{\text{NS}}(Q^2/\mu^2, a_s(\mu^2)) + C_{\text{GLS}}^{\text{S}}(Q^2/\mu^2, a_s(\mu^2)) \quad (2.11)$$

As a consequence of the chiral invariance, which can be restored in the dimensional regularization [39] by means of additional finite renormalizations (for their consequent evaluation in high-loop orders see, e.g., [37, 38, 40, 41]), the NS contributions to the leading twist coefficient function of $S_{\text{GLS}}(Q^2)$ coincide with a similar NS perturbative contribution $S^{\text{Bjp}}(Q^2)$, namely

$$\begin{aligned} C_{\text{GLS}}^{\text{NS}}(Q^2/\mu^2, a_s(\mu^2)) &\equiv C_{\text{NS}}^{\text{Bjp}}(Q^2/\mu^2, a_s(\mu^2)) = 1 + \sum_{l \geq 1} c_l^{\text{NS}}(Q^2/\mu^2) a_s^l(\mu^2) \\ &\xrightarrow{\mu^2=Q^2} C_{\text{NS}}^{\text{Bjp}}(a_s(Q^2)) = 1 + \sum_{l \geq 1} c_l^{\text{NS}} a_s^l(Q^2). \end{aligned} \quad (2.12)$$

The fulfilment of this identity was explicitly demonstrated in the existing analytical NLO and N²LO calculations in [37, 38] and used as the input in the process of determination of the analytical expression for the $\mathcal{O}(a_s^4)$ corrections to $S_{\text{GLS}}(Q^2)$ [34].

The second (singlet-type) contribution to the coefficient function of Eq.(2.11) has the following form:

$$\begin{aligned} C_{\text{GLS}}^{\text{S}}(Q^2/\mu^2, a_s(\mu^2)) &= n_f \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} \bar{c}_l(Q^2/\mu^2) a_s^l(\mu^2) \\ &\xrightarrow{\mu^2=Q^2} C_{\text{GLS}}^{\text{S}}(a_s(Q^2)) = n_f \frac{d^{abc} d^{abc}}{d_R} \sum_{l \geq 3} \bar{c}_l a_s^l(Q^2) \end{aligned} \quad (2.13)$$

where \bar{c}_3 and \bar{c}_4 were evaluated analytically in [38] and [34], respectively.

The application of the OPE approach to the three-point functions of axial-vector-vector currents (see [30–32, 35, 36]) leads to the following $\overline{\text{MS}}$ -scheme QCD generalization of the Crewther relation (CR) between the introduced above different coefficient functions of the annihilation and deep-inelastic scattering processes:

$$C^{\text{Bjp}}(a_s)D^{\text{NS}}(a_s) \equiv C_{\text{GLS}}(a_s)[D^{\text{NS}}(a_s) + n_f D^{\text{S}}(a_s)] \quad (2.14a)$$

$$= \mathbb{1} + \frac{\beta(a_s)}{a_s} \cdot K(a_s), \quad (2.14b)$$

where $\mathbb{1}$ was derived in [27] using the conformal symmetry, $\beta(a_s)$ is the RG β -function, $a_s = a_s(Q^2)$ and the polynomial K is

$$K(a_s) = a_s K_1 + a_s^2 K_2 + a_s^3 K_3 + O(a_s^4). \quad (2.15)$$

It contains the coefficients K_1 and K_2 , obtained in [29], while the analytical expression for the coefficient $K_3 = K_3^{\text{NS}} + K_3^{\text{S}}$ is the sum of the NS- and S-terms, which are given in [33] and [34], respectively. Note that Eq.(2.14a) was first published in [35] without taking into account singlet-type contributions to C^{Bjp} . Their more careful analysis of [36] fixes the β_0 -dependent analytical expression of the $\mathcal{O}(a_s^4)$ contribution to C_S^{Bjp} ².

The result of [36] and the general Eq.(2.14a) is not yet confirmed by direct analytical calculations. In our further studies we will use the product of their NS parts and related to this product results of the expansion in Eq.(2.14b), reformulated in [9].

3. GENERAL β -EXPANSION STRUCTURE OF OBSERVABLES

1. Formulation of the approach

To clarify the main ideas of the $\{\beta\}$ -expansion representation proposed in [8] for the perturbative coefficients of the RGI quantities, let us consider the NS part of the Adler function, D^{NS} . Its expression can be rewritten as $D^{\text{NS}} = 1 + d_1^{\text{NS}} \cdot \sum_{n \geq 1} d_n a_s^n$, where $d_1^{\text{NS}} = 3C_F$ is the overall normalization factor. Within the $\{\beta\}$ -expansion approach the coefficients d_n , originally fixed in the $\overline{\text{MS}}$ -scheme, are expressed as

$$d_1 = d_1[0] = 1, \quad (3.1a)$$

$$d_2 = \beta_0 d_2[1] + d_2[0], \quad (3.1b)$$

$$d_3 = \beta_0^2 d_3[2] + \beta_1 d_3[0, 1] + \beta_0 d_3[1] + d_3[0], \quad (3.1c)$$

$$d_4 = \beta_0^3 d_4[3] + \beta_1 \beta_0 d_4[1, 1] + \beta_2 d_4[0, 0, 1] + \beta_0^2 d_4[2] + \beta_1 d_4[0, 1] + \beta_0 d_4[1] + d_4[0], \quad (3.1d)$$

\vdots

$$d_N = \beta_0^{N-1} d_N[N-1] + \dots + d_N[0], \quad (3.1e)$$

where the first argument of the expansion elements $d_n[n_0, n_1, \dots]$ indicates its multiplication to the n_0 -th power of the first coefficient β_0 of the RG β -function, namely to the $\beta_0^{n_0}$

² In QED the validity of Eq.(2.14a) follows from the considerations of Ref. [42].

term. The second argument n_1 determines the power of the second multiplication factor, namely $\beta_1^{n_1}$, and so on. The elements $d_n[0] \equiv d_n[0, 0, \dots, 0]$ define “refined” β_i -independent corrections with powers $n_i = 0$ of all their $\beta_i^{n_i}$ multipliers. These elements coincide with expressions for the coefficients d_n in the imaginary situation of the nullified QCD β -function in all orders of perturbation theory. This case corresponds to the effective restoration of the conformal symmetry limit of the bare $SU(N_c)$ model in the case when all normalizations are not considered. This limit, extensively discussed in [17], will be considered here as a technical trick. The origins of other elements in Eqs. (3.1) were considered in [8].

The first elements $d_i[i-1]$ of the expansions of Eqs.(3.1b-3.1e) arise from the diagrams with a maximum number of the “fermion 1-loop bubble” insertions and applications of the Naive Non-Abelianization (NNA) approximation [43]). In the case of D^{NS} -function they can be obtained from the result in [29], which follow from renormalon-type calculations in [44, 45].

It would be stressed that the terms $\beta_0 d_3[1]$, $\beta_1 d_4[0, 1]$, $\beta_0 d_4[1]$ in Eqs.(3.1) were not taken into account in the variant of the $\{\beta\}$ -expansion method used in [4–6]. The omitting of these terms leads to the results, which should be corrected by including these terms in the self-consistent variant of the PMC analysis.

In high order of perturbation theory one should also consider a similar expression of the singlet part $D^{\text{S}} = d_3^{\text{S}} \cdot \sum_{j \geq 3} \bar{d}_j a_s^{(j)}$ with the normalization factor $d_3^{\text{S}} = 11/3 - 8\zeta_3$ evaluated first in the QED work [46], and the related normalizations of the defined coefficients in Eq.(2.13), namely $\bar{d}_j = d_j^{\text{S}}/d_3^{\text{S}}$. The $\{\beta\}$ -expanded coefficients of this RGI-invariant quantity are expressed as

$$\bar{d}_3 = \bar{d}_3[0] = 1 \quad (3.2a)$$

$$\bar{d}_4 = \beta_0 \bar{d}_4[1] + \bar{d}_4[0], \quad (3.2b)$$

$$\vdots$$

$$\bar{d}_{j+2} = \beta_0^{j-1} \bar{d}_{j+2}[j-1] + \dots + \bar{d}_{j+2}[0]. \quad (3.2c)$$

The same ordering in the β -function coefficients can be applied to the coefficients c_n for the NS coefficient function of the deep-inelastic sum rules C^{NS} of Eq.(2.12) and to the singlet contribution C^{S} to the GLS sum rule (see Eq. (2.13). Moreover, it is possible to show that the elements of the corresponding $\{\beta\}$ -expansions $d_n[n_0, n_1, \dots]$ and $c_n[n_0, n_1, \dots]$ are closely related [9]. We will return to a more detailed discussion of this property a bit later.

The above $\{\beta\}$ -expansion can be interpreted as a “matrix” representation for the RGI quantities: For the quantity D^{NS} expanded up to an order of N , $D^{\text{NS}} = \sum_{n=1}^N a_s^n \sum_{i \geq 0} D_{ni}^{\text{NS}} B^{(i)}$ which is related to the traditional “vector” representation, $D^{\text{NS}} = \sum_{n=1}^N a_s^n d_n$ with $d_n = \sum_i D_{ni}^{\text{NS}} B^{(i)}$. Here $B^{(i)}$ are the elements that express the structure of $\{\beta\}$ -expanded perturbative coefficients and are convolved with the matrix elements $D_{ni}^{\text{NS}} = d_n[\dots]$. In the case of consideration of the “refined” β_i -independent corrections $d_n[0] \equiv D_{n0}$ and $B^{(0)} = 1$. The similar matrix representation can be written down for the singlet part D^{S} with the $\{\beta\}$ -expanded coefficient defined in Eqs.(3.2a-3.2c).

Note that the matrix representation contains new dynamical information about the RGI invariant quantities, which is not contained in the vector one. Thus, Eqs. (3.1b),(3.2b) can be considered as the initial points to apply the standard BLM procedure. The generalization of the BLM procedure to higher orders can be constructed using the $\{\beta\}$ -expansions of higher order coefficients of Eqs. (3.1) [8]. However, starting with the N²LO the explicit solution of this problem is nontrivial.

2. Explicit determination of the structures of the $\{\beta\}$ -expanded series for D^{NS}

Let us start the discussion of application of the $\{\beta\}$ -expansion procedure in the NLO. Imagine that we deal with the perturbative quenched QCD (pqQCD) approximation for the D^{NS} -function in the NLO. It is described by the contributions of the three-loop photon vacuum polarization diagrams with closed external loop, formed by quark-antiquark pair and connected by internal gluon propagators, which do not contain any internal quark-loop insertions. In this theoretical approximation the coefficient d_2 takes the following form:

$$d_2 \rightarrow d_2^{pqQCD} = -\frac{C_F}{2} + \left(\frac{123}{2} - 44\zeta_3 \right) \frac{C_A}{3} \text{ with } \beta_0 = \frac{11}{3}C_A. \quad (3.3)$$

In this case, it is unclear how to perform the standard BLM scale-fixing prescription in the NLO approximation. Indeed, it is not clear what is the expression for the $d_2[1]$ coefficient of the β_0 -term of Eq.(3.1b) in the expression for d_2^{pqQCD} . To obtain explicitly the elements of the expansion (3.1b) and extract the β_0 -term in (3.3), one should take into account the quark-antiquark one-loop insertion in internal gluon lines of the three-loop approximation for the hadronic vacuum polarization function. This is equivalent to taking into account in the pqQCD model of the interacting with gluons of internal quark loops with \mathbf{n}_f number of active quarks. The corresponding parameter \mathbf{n}_f can be considered as *a mark* of the charge renormalization by the quark-antiquark pair. It enters into both d_2 and β_0 expressions and allows one to extract *unambiguously* the expression for d_2 proportional to the β_0 -term in the $\overline{\text{MS}}$ -scheme. Indeed, fixing $T_R = T_F = \frac{1}{2}$ we obtain

$$d_2 = -\frac{C_F}{2} + \left(\frac{11 \cdot 11 + 2}{2} - 44\zeta_3 \right) \frac{C_A}{3} - \left(\frac{11}{2} - 4\zeta_3 \right) \frac{2}{3} \mathbf{n}_f \text{ with } \beta_0 = \frac{11}{3}C_A - \frac{2}{3} \mathbf{n}_f. \quad (3.4)$$

To get the appropriate expression of the coefficient d_2 one should take into account the 1-loop renormalization of charge. As the result, we immediately obtain from Eq. (3.4) the following expression for the coefficient of Eq.(3.1b):

$$d_2 = \frac{C_A}{3} - \frac{C_F}{2} + \left(\frac{11}{2} - 4\zeta_3 \right) \left(\frac{11}{3}C_A - \frac{2}{3} \mathbf{n}_f \right) \quad (3.5a)$$

where

$$d_2[0] = \frac{C_A}{3} - \frac{C_F}{2}, \quad d_2[1] = \frac{11}{2} - 4\zeta_3 \quad . \quad (3.5b)$$

This decomposition corresponds to the case of the standard BLM consideration in the $\overline{\text{MS}}$ -scheme [2]. Note that for $\mathbf{n}_f = 0$ this decomposition remains valid for the case of pqQCD (QCD at $\mathbf{n}_f = 0$) and leads to Eq.(3.5b).

Any additional modifications of QCD, say, by means of introducing into considerations $\mathbf{n}_{\tilde{g}}$ multiplets of strong interacting gluino (the element of the MSSM model), will change in the NLO expression for the considered RGI invariant quantity the content of the β_0 -coefficient in the expression for d_2 , calculated in the $\overline{\text{MS}}$ -scheme, but not the “refined” element and the coefficients at β_0 of Eq.(3.3). Using the result β_0 for the β -function with the $\mathbf{n}_{\tilde{g}}$ multiplet of strong interacting gluino (see Eq. (A.1a)) and the D^{NS} -function in the same model (presented in Eq.(A.5b) of the Appendix A), the same result (3.5b) for decomposition can

unambiguously be obtained using the additional *marks* in Eq.(3.5a), namely the number of strong-interacting gluino $\mathbf{n}_{\tilde{g}}$. Indeed, combining the result

$$d_2 = \frac{C_A}{3} - \frac{C_F}{2} + \left(\frac{11}{2} - 4\zeta_3\right) \left(\frac{11}{3}C_A - \frac{2}{3}\mathbf{n}_f\right) - (11 - 8\zeta_3)\mathbf{n}_{\tilde{g}}\frac{C_A}{3}, \quad (3.6a)$$

with

$$\beta_0(\mathbf{n}_f, \mathbf{n}_{\tilde{g}}) = \frac{11}{3}C_A - \frac{2}{3}(\mathbf{n}_f + \mathbf{n}_{\tilde{g}}C_A) \quad (3.6b)$$

we get the expressions for $d_2[0]$ and $d_2[1]$, which are identical to the ones presented in Eq.(3.5b). Note that these results can be obtained from Eq.(3.6a) and Eq.(3.6b) with gluino degrees of freedom only ($\mathbf{n}_{\tilde{g}} \neq 0$, $\mathbf{n}_f = 0$), or only with the quark ones ($\mathbf{n}_f \neq 0$, $\mathbf{n}_{\tilde{g}} = 0$), or with taking into account both of them. The reason of this unambiguity is that the interaction of any new particle accumulated here in the charge renormalization is determined by the universal gauge group $SU(N_c)$.

All these possibilities give us a simple tool to restore the β_0 -term in the NLO following the BLM prescription [2]. Thus, in the NLO we may switch off the gluino degrees of freedom. However, to get the $\{\beta\}$ expansion of the N²LO term in the form of Eq. (3.1c) we cannot use the quark degrees of freedom only. Indeed, in this case, we face a problem similar to that which arises in the process of $\{\beta\}$ decomposition of the pqQCD expression for d_2^{pqQCD} in Eq. (3.3) discussed above.

The $\{\beta\}$ -expanded form for the d_3 -term was obtained in Ref. [8] by means of a careful consideration of the analytical $\mathcal{O}(a_s^3)$ $\overline{\text{MS}}$ -scheme expression for the Adler function $D^{\text{NS}}(a_s, \mathbf{n}_f, \mathbf{n}_{\tilde{g}})$ with the $\mathbf{n}_{\tilde{g}}$ QCD interacting MSSM gluino multiplets obtained in [25] and presented in Eq. (A.5)³ together with the corresponding two-loop β -function, $\beta(\mathbf{n}_f, \mathbf{n}_{\tilde{g}})$, see Eqs. (A.1a, A.1b).

Let us consider this procedure in more detail. The element $d_3[2]$, which is proportional to the maximum power β_0^2 in (3.1c), can be fixed in a straightforward way, using the results in [29]. Then one should separate the contributions of $\beta_1 d_3[0, 1]$ and of $\beta_0 d_3[1]$ to the d_3 -term. They both are linear in the number of quark flavours \mathbf{n}_f , therefore, they could not be disentangled directly. Their separation is possible if one takes into account additional degrees of freedom, *e.g.*, the gluino contributions mentioned above for both the quantities (the additional *mark* appears), namely for the D^{NS} -function from Eqs.(A.8c) and for the first two coefficients of the β -function from Eqs.(A.1a, A.1b). In this way, using two equations one can get the explicit form for the functions $\mathbf{n}_f = n_f(\beta_0, \beta_1)$ and $\mathbf{n}_{\tilde{g}} = n_{\tilde{g}}(\beta_0, \beta_1)$. Finally, substituting these functions in $D = D(a_s, n_f(\beta_0, \beta_1), n_{\tilde{g}}(\beta_0, \beta_1))$ its $\{\beta\}$ -expanded expression was obtained in [8],

$$\begin{aligned} D^{\text{NS}}(a_s, n_f, n_{\tilde{g}}) = & 1 + a_s(3C_F) + a_s^2(3C_F) \cdot \left\{ \frac{C_A}{3} - \frac{C_F}{2} + \left(\frac{11}{2} - 4\zeta_3\right) \beta_0(n_f, n_{\tilde{g}}) \right\} \\ & + a_s^3(3C_F) \cdot \left\{ \left(\frac{302}{9} - \frac{76}{3}\zeta_3\right) \beta_0^2(n_f, n_{\tilde{g}}) + \left(\frac{101}{12} - 8\zeta_3\right) \beta_1(n_f, n_{\tilde{g}}) \right. \\ & + \left[C_A \left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5\right) - C_F(18 + 52\zeta_3 - 80\zeta_5) \right] \beta_0(n_f, n_{\tilde{g}}) \\ & \left. + \left(\frac{523}{36} - 72\zeta_3\right) C_A^2 + \frac{71}{3}C_A C_F - \frac{23}{2}C_F^2 \right\}, \end{aligned} \quad (3.7a)$$

³ The evaluated in [25] N²LO analytical result for the gluino contribution was confirmed in [47].

with (see Eqs.(A.1) in AppendixA)

$$\beta_1(n_f, n_{\tilde{g}}) = \frac{34}{3}C_A^2 - \frac{20}{3}C_A \left(T_R n_f + \frac{n_{\tilde{g}} C_A}{2} \right) - 4 \left(T_R n_f C_F + \frac{n_{\tilde{g}} C_A}{2} C_A \right). \quad (3.7b)$$

Note that in order to write down the $\mathcal{O}(a_s^4)$ coefficient of D^{NS} , analytically evaluated in the $\overline{\text{MS}}$ -scheme in [33] for the case of $SU(N_c)$ in a similar $\{\beta\}$ -expanded form of Eq.(3.1d), it is necessary to perform additional calculations, which generalize this result to the case of $SU(N_c)$ with $n_{\tilde{g}}$ multiplets of gluino. Then, one should combine this possible (but not yet existing) generalization with already available analytical expression for the $\beta_2(n_f, n_{\tilde{g}})$ -coefficient of the β -function in this model, analytically obtained in the $\overline{\text{MS}}$ -scheme in [48].

3. Does $\{\beta\}$ -expansion have any ambiguities ?

It is instructive to discuss here an attempt [5, 7] to obtain the elements $d_n[\dots]$ in a different way. This is based on the expression for D , rewritten in [49] for the usability of current 5-loop computation in the form

$$D^{\text{EM}}(a_s) = 12\pi^2 \left(\gamma_{\text{ph}}^{\text{EM}}(a_s) - \beta(a_s) \frac{d}{da_s} \Pi^{\text{EM}}(a_s) \right). \quad (3.8)$$

Here $\Pi^{\text{EM}}(a_s) = \Pi^{\text{EM}}(L, a_s) \equiv d_R/(4\pi)^2 \sum_{i \geq 0} \Pi_i a_s^i$ is the polarization function of electromagnetic currents at $L \equiv \ln(Q^2/\mu^2) = 0$, and $\gamma_{\text{ph}}^{\text{EM}} \equiv 1/(4\pi)^2 \sum_{j \geq 0} \gamma_j a_s^j$ is the anomalous dimension of the photon field. In our notation Eq. (3.8) leads to the expansion for D^{NS} ,

$$D^{\text{NS}}(a_s) = 1 + 3C_F a_s + (12\gamma_2 + 3\beta_0 \Pi_1) a_s^2 + (48\gamma_3 + 3\beta_1 \Pi_1 + 24\beta_0 \Pi_2) a_s^3 + \dots, \quad (3.9)$$

where the ingredients of the expansion, γ_i , Π_j , were calculated in [49] up to $i = 4$, $j = 3$, and we take corresponding NS projection in the RHS of Eq.(3.8). The renormalization of the charge certainly contributes to the 3-loop anomalous dimension γ_2 ; therefore, it contains a β_0 -term also (one can make sure from the inspection of the explicit formula for γ_2 in Eq. (3.12) in [49] and even in Eq.(10) in [20]). Taking into account the explicit form of γ_2 and Π_1 in (3.9) one can recalculate the well-known decomposition for D^{NS} in order $\mathcal{O}(a_s^2)$

$$D^{\text{NS}}(a_s) = 1 + 3C_F \cdot a_s + 3C_F \cdot (\beta_0 d_2[1] + d_2[0]) a_s^2 + \mathcal{O}(a_s^3) \quad (3.10)$$

in full accordance with the result in [2] and Eq. (3.1b) (for the related discussions see Ref. [17] as well).

Unfortunately the authors of [7] claim, basing on a formal correspondence, that the coefficient of β_0 is only the term Π_1/C_F in Eq. (3.9) (with the above notation at d_1 normalized by unity), while the “conformal term” is $4\gamma_2/C_F$ (see Eq. (48a-b) in [2]), which in reality is not true. The comparison of these terms

$$d_2[1] = \frac{11}{2} - 4\zeta_3 \approx 0.69177 \quad \Leftrightarrow \quad \Pi_1/C_F = \frac{55}{12} - 4\zeta_3 \approx -0.22489; \quad (3.11)$$

$$d_2[0] = d_2[0] = \frac{C_A}{3} - \frac{C_F}{2} \quad \Leftrightarrow \quad 4\gamma_2/C_F = \frac{11}{12}\beta_0 - \frac{C_F}{2} \quad (3.12)$$

shows that they differ even in sign in (3.11) [compare Π_1/C_F with $d_2[1]$]. The considerations of the lead to a shift of the BLM scale Q_{BLM}^2 in the opposite direction, $Q_{\text{BLM}}^2 \geq Q^2$, in comparison with the standard value $Q_{\text{BLM}}^2 = \exp(-d_2[1]) Q^2 \approx Q^2/2$ (see the discussion after Eq. (5.3g) in Sec.5). Moreover, we demonstrate in Eq.(3.12) that γ_2 is not “conformal” and depends on β_0 .

4. PARTIAL β -EXPANSION ELEMENTS FOR D , C , AND R

Here we extend our knowledge about the β -expansion elements on NS part of the Bjorken C^{Bjp} basing on CR Eq.(2.14b) for D^{NS} and $C_{\text{NS}}^{\text{Bjp}}$.

1. What constraints Crewther relation gives

In the case **of** the β -function has identically zero coefficients $\beta_i = 0$ for $i \geq 0$ the generalized CR (2.14b) returns to its initial form [27]

$$D_0^{\text{NS}} \cdot C_0^{\text{Bjp}} = \mathbb{1}, \quad (4.1)$$

where the expansions for the functions D_0^{NS} and C_0^{Bjp} , analogous to the ones of Eq. (3.1b-3.1e), contain the coefficients of genuine content only, namely, d_n (c_n) $\equiv d_n[0]$ ($c_n[0]$). Equation (4.1) provides an evident relation between the genuine elements in any loops, namely,

$$c_n^{\text{NS}}[0] + d_n^{\text{NS}}[0] + \sum_{l=1}^{n-1} d_l^{\text{NS}}[0] c_{n-l}^{\text{NS}}[0] = 0, \quad (4.2)$$

where $d_n^{\text{NS}}[0] = d_1^{\text{NS}} \cdot d_n[0]$ and $c_n^{\text{NS}}[0] = c_1^{\text{NS}} \cdot c_n[0]$ in virtue of the normalization condition. From Eq. (4.2) at $n = 1$ immediately follows that $c_1^{\text{NS}} = -d_1^{\text{NS}}$. The relation (4.2) can be used to obtain the unknown genuine parts of the 4-loop term $c_3^{\text{NS}}[0]$, through the 4-loop results already known from the analysis in [8]:

$$c_3^{\text{NS}}[0] = -d_3^{\text{NS}}[0] + 2d_1^{\text{NS}}d_2^{\text{NS}}[0] - (d_1^{\text{NS}})^3, \quad (4.3a)$$

or, in the other normalized terms,

$$c_3[0] = d_3[0] - 2d_1^{\text{NS}}d_2[0] + (d_1^{\text{NS}})^2, \quad (4.3b)$$

It is useful to relate the unknown elements $c_4^{\text{NS}}[0], d_4^{\text{NS}}[0]$ in a 5-loop calculation with the known elements of the 4-loop results, viz,

$$c_4^{\text{NS}}[0] + d_4^{\text{NS}}[0] = 2d_1^{\text{NS}}d_3^{\text{NS}}[0] - 3(d_1^{\text{NS}})^2d_2^{\text{NS}}[0] + (d_2^{\text{NS}}[0])^2 + (d_1^{\text{NS}})^4. \quad (4.4)$$

Let us consider now the generalized CR in Eq.(2.14b), which includes the terms proportional to the conformal anomaly, $\beta(a_s)/a_s$, appearing due to violation of the the conformal symmetry in the renormalized $\text{SU}(N_c)$ interaction (in the $\overline{\text{MS}}$ -scheme). As was shown in [9], this relation can be rewritten in the following multiple power representation:

$$D^{\text{NS}} \cdot C_{\text{NS}}^{\text{Bjp}} = \mathbb{1} + \frac{\beta(a_s)}{a_s} \cdot K(a_s) = \mathbb{1} + \frac{\beta(a_s)}{a_s} \cdot \sum_{n \geq 1} \left(\frac{\beta(a_s)}{a_s} \right)^{n-1} \mathcal{P}_n(a_s), \quad (4.5)$$

where $\mathcal{P}_n(a_s)$ are the polynomials in a_s that can be expressed only in terms of the elements $d_k[\dots]$, $c_k[\dots]$. In this sense \mathcal{P}_n do not depend on the β -function, all the charge renormalizations being accumulated by $(\beta(a_s)/a_s)^n$. Below we present the first two polynomials (factor

$$\text{out } -c_1^{\text{NS}} = d_1^{\text{NS}} = 3C_F)$$

$$\mathcal{P}_1(a_s) = -a_s d_1^{\text{NS}} \left\{ d_2[1] - c_2[1] + a_s [d_3[1] - c_3[1] - d_1^{\text{NS}}(d_2[1] + c_2[1])] \right. \quad (4.6a)$$

$$\left. + a_s^2 [d_4[1] - c_4[1] - d_1^{\text{NS}} (d_3[1] + c_3[1] + d_2[0]c_2[1] + d_2[1]c_2[0])] \right\}, \quad (4.6b)$$

$$\mathcal{P}_2(a_s) = a_s d_1^{\text{NS}} \left\{ d_3[2] - c_3[2] + a_s [d_4[2] - c_4[2] + d_1^{\text{NS}} (c_3[2] + d_3[2])] \right\}, \quad (4.6c)$$

which were obtained and verified in N³LO in [9, 10] in another normalization. The construction of the β -term in the RHS of (4.5) also creates constraints for combinations of the β -expansion elements. A few chains of these constraints were obtained in [9]. Further we shall use the relation

$$d_2[1] - c_2[1] = d_3[0, 1] - c_3[0, 1] = \dots = d_n[\underbrace{0, 0, \dots, 1}_{n-1}] - c_n[\underbrace{0, 0, \dots, 1}_{n-1}] = \left(\frac{7}{2} - 4\zeta_3 \right), \quad (4.7)$$

that corresponds to Eq.(30) in [9].

If the terms $c_3[1]$, $d_3[1]$ and $c_4[2]$, $d_4[2]$ are missed in the $\{\beta\}$ -expansion of D^{NS} and $C_{\text{NS}}^{\text{Bjp}}$, as in the variant of the expansion in [4–7], the structure of the generalized CR in (4.6) is corrupted. That structure certainly contradicts the explicit results of analytical calculations of $D^{\text{NS}}(a_s)$ and $C_{\text{NS}}^{\text{Bjp}}(a_s)$, preformed in the N²LO in [23–25] and in N³LO in [33].

2. Nonsinglet parts of D and C^{Bjp}

Following the approach discussed in Sec. 3 and taking into account a certain definition of the β -function coefficients in Eq. (2.3) we can obtain the β -expansion for D - and C -functions. For the Adler function D^{NS} it reads

$$d_1^{\text{NS}} = 3C_F; \quad d_1 = 1; \quad (4.8a)$$

$$d_2[1] = \frac{11}{2} - 4\zeta_3; \quad d_2[0] = \frac{C_A}{3} - \frac{C_F}{2} = \frac{1}{3}; \quad (4.8b)$$

$$d_3[2] = \frac{302}{9} - \frac{76}{3}\zeta_3 \approx 3.10345; \quad d_3[0, 1] = \frac{101}{12} - 8\zeta_3 \approx -1.19979; \quad (4.8c)$$

$$d_3[1] = C_A \left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5 \right) - C_F (18 + 52\zeta_3 - 80\zeta_5) \approx 55.7005; \quad (4.8d)$$

$$d_3[0] = \left(\frac{523}{36} - 72\zeta_3 \right) C_A^2 + \frac{71}{3} C_A C_F - \frac{23}{2} C_F^2 \approx -573.9607, \quad (4.8e)$$

which differs from the ones presented in Ref. [9] (see its “natural form” in the Appendix B), by the normalization factor only. It looks more convenient for a certain BLM task (the presentation corresponds to one in [8]) due to setting of the first PT coefficient, d_1 (c_1), equal to 1. Let us emphasize that gluinos are used here as a pure technical device to reconstruct the β -function expansion of the perturbative coefficients.

In this connection, we mention the relation $d_3[0, 1] = d_n[0, \dots, 1] = d_2[1]$ proposed in [5] and based on a “special degeneracy of the coefficients” suggested there (see Eq. (6) in [5])

in an analogy with the perturbative series rearrangement, $d_i \rightarrow d'_i$ under the change of the coupling renormalization scale, $a(\mu^2) \rightarrow a'(\mu'^2)$ (see below the discussions around Eq. (5.3)). This rearrangement has an *outside* reason with respect to d_i and “does not know” about the *intrinsic* structure of the initial coefficient d_i under consideration. This relation is artificial and by this reason it is not supported by the direct calculations. The explicit result of this rearrangement is presented in Eq. (5.3), it is the initial step for any BLM optimization procedure that will be discussed in Sec.5 in detail.

Let us compare now Eqs. (4.8) with the results presented in [7] and based on the interpretation of the term $(48\gamma_3 + 3\beta_1\Pi_1 + 24\beta_0\Pi_2) a_s^3$ in the presentation of (3.9). The first and the third terms of the sum form the term proportional to β_0^2

$$\underline{48\gamma_3} + \underline{24\beta_0\Pi_2} \longrightarrow \beta_0^2 \left(\frac{302}{9} - \frac{76}{3}\zeta_3 = d_3[2] \right) \quad (4.9)$$

that can be unambiguously obtained by extracting the n_f^2 terms in γ_3 and the β_0 -term in Π_2 , see the corresponding explicit expressions in [49]. The second term there, $\beta_1\Pi_1$, certainly contributes to the value of the element $d_3[0, 1]$. There are other terms, proportional to β_1 , in both the γ_3 and $\beta_0\Pi_2$ terms that also contribute to $d_3[0, 1]$. However, these required terms cannot be separated unambiguously from those terms that are proportional to β_0 . The final explicit expressions given in [49] are not sufficient for this separation, as it was already discussed in Subsec.3.2.

Let us consider the β -expansion of the Bjorken coefficient function $C_{\text{NS}}^{\text{Bjp}}$ of the DIS sum rules. Based on CR (4.2) for $n = 2$ and $n = 3$ and the already fixed $d_2[0]$ and $d_3[0]$ -terms we get expression (4.3b) for the $c_2[0]$ and $c_3[0]$ elements of $C_{\text{NS}}^{\text{Bjp}}$, namely, $c_3[0] = d_3[0] - 2d_1^{\text{NS}}d_2[0] + (d_1^{\text{NS}})^2$, see the explicit expression in (4.10e). The knowledge of $c_3[0]$ allowed us to fix all other elements $c_3[\dots]$ of the PT coefficient c_3 without involving additional degrees of freedom [9]. It is instructive to consider this in detail. Indeed, the terms $c_3[0]$ as well as the coefficient $c_3[2]$ of the β_0^2 (maximum power of n_f) can be found independently. Therefore, the Casimir structure of the rest of c_3 , $c_3 - c_3[0] - \beta_0^2 c_3[2]$, contains **5** basis elements (we factor out $c_1^{\text{NS}} = -3C_F$):

$$c_3 - c_3[0] - \beta_0^2 c_3[2] : \left\{ \begin{array}{l} C_F^2, C_A^2, C_A C_F, T_R n_f C_F, T_R n_f C_A \\ \beta_1, \beta_0 \end{array} \right.$$

This Casimir expansion of the rest should be equated to the β -expansion of the one (see decomposition (3.1)), $c_3[0, 1] \cdot \beta_1 + (x \cdot C_F + y \cdot C_A) \cdot \beta_0$ that contains 3 unknown coefficients $c_3[0, 1], x, y$.

The C_F^2 -terms in the explicit result for c_3 [38] (see App.A, Eq.(A.7)) and in the expression for $c_3[0]$ in Eq.(4.10e) coincide to one another; therefore, the term $\frac{1}{2}C_F^2$ is canceled in the rest. This confirms the fact that its β -expansion does not contain C_F^2 . So we have **4** constraints (not **5**) for the **3** coefficients $c_3[0, 1], x, y$. This overdetermined system is a system of simultaneous equations; the fact provides us with an *independent confirmation* of this β -expansion. The explicit form of the elements were first obtained in [9]; below we present them at the same normalization as Eq. (4.8) (cf. (4.8e) with (4.10e)):

$$c_1^{\text{NS}} = -3 C_F; \quad c_1 = 1; \quad (4.10a)$$

$$c_2[1] = 2; \quad c_2[0] = \left(\frac{1}{3}C_A - \frac{7}{2}C_F \right) = -\frac{11}{3} = -3.6(6); \quad (4.10b)$$

$$c_3[2] = \frac{115}{18} = 6.38(8); \quad c_3[0, 1] = \left(\frac{59}{12} - 4\zeta_3 \right) \approx 0.10844; \quad (4.10c)$$

$$c_3[1] = -\left(\frac{166}{9} - \frac{16}{3}\zeta_3 \right) C_F - \left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5 \right) C_A \approx 39.9591; \quad (4.10d)$$

$$c_3[0] = \left(\frac{523}{36} - 72\zeta_3 \right) C_A^2 + \frac{65}{3} C_F C_A + \frac{C_F^2}{2} \approx -560.627. \quad (4.10e)$$

The same results can be obtained if one fixes first the element $c_3[0, 1] = d_3[0, 1] - d_2[1] + c_2[1]$ from relation (4.7), the latter originates from another source – the symmetry breaking term proportional to $\beta(a_s)$ in the generalized CR. Therefore, the results (4.10) are in mutual agreement with both the terms in the RHS of CR and can be obtained independently from each of them.

These elements of decomposition in (4.10) allows one to make a *new prediction* for the light gluino contribution to $C_{\text{NS}}^{\text{Bjp}}$. Indeed, for the considered here RGI quantities the effects of charge renormalization appear in two ways: the elements $c[\dots]$ – the coefficients of the β -function products (named B^j in 3.1) – are formed following gauge interaction; the effect of various degrees of freedom, say, gluino, which reveals itself only in intrinsic loops, changes the content of the β -coefficients β_i with the corresponding mark, say, $\mathbf{n}_{\tilde{g}}$. Therefore, to obtain $C^{\text{Bjp}} \rightarrow C^{\text{Bjp}}(a_s, n_f, n_{\tilde{g}})$ with the light MSSM gluino one should replace the β -coefficients $\beta_i \rightarrow \beta_i(n_f, n_{\tilde{g}})$ and compose them with the elements from Eq.(4.10),

$$C_{\text{NS}}^{\text{Bjp}}(a_s, n_f, n_{\tilde{g}}) = 1 + a_s(-3C_F) \quad (4.11a)$$

$$+ a_s^2(-3C_F) \cdot \left\{ \frac{1}{3}C_A - \frac{7}{2}C_F + 2\beta_0(n_f, n_{\tilde{g}}) \right\} \quad (4.11b)$$

$$+ a_s^3(-3C_F) \cdot \left\{ \frac{115}{18}\beta_0^2(n_f, n_{\tilde{g}}) + \left(\frac{59}{12} - 4\zeta_3 \right) \beta_1(n_f, n_{\tilde{g}}) \right. \\ \left. - \left[\left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5 \right) C_A + \left(\frac{166}{9} - \frac{16}{3}\zeta_3 \right) C_F \right] \beta_0(n_f, n_{\tilde{g}}) \right. \\ \left. + \left(\frac{523}{36} - 72\zeta_3 \right) C_A^2 + \frac{65}{3} C_F C_A + \frac{C_F^2}{2} \right\}. \quad (4.11c)$$

This logic can be reverted: the values of $c_3[0]$, $c_3[0, 1]$ and then the CR can be checked from the direct calculation of $C_{\text{NS}}^{\text{Bjp}}(a_s, n_f, n_{\tilde{g}})$ with the MSSM massless gluino.

3. Singlet parts and the R -ratio

Here we present the singlet part of the Adler function, d_4 , that can be obtained based on the result for c_4 of C_S^{Bjp} and CR [34],

$$d_4^S = \beta_0(n_f) \cdot d_4^S[1] + d_4^S[0], \quad (4.12)$$

$$d_4^S[0] = \left(-\frac{13}{64}\zeta_3 - \frac{5}{32}\zeta_5 + \frac{205}{1536} \right) C_A + \left(-\frac{1}{4}\zeta_3 + \frac{5}{8}\zeta_5 - \frac{13}{64} \right) C_F, \quad (4.13)$$

$$d_4^S[1] = -\frac{13}{32}\zeta_3 - \frac{1}{8}\zeta_3^2 + \frac{5}{16}\zeta_5 + \frac{149}{576}, \quad (4.14)$$

$$c_4^S = c_4^S[0] + \beta_0(n_f) \cdot c_4^S[1], \quad (4.15)$$

$$c_4^S[0] = \left(\frac{13}{64}\zeta_3 + \frac{5}{32}\zeta_5 - \frac{205}{1536} \right) C_A + \left(\frac{1}{16}\zeta_3 - \frac{5}{8}\zeta_5 + \frac{37}{128} \right) C_F, \quad (4.16)$$

$$c_4^S[1] = -\frac{119}{1152} + \frac{67}{288}\zeta(3) + \frac{1}{8}\zeta(3)^2 - \frac{35}{144}\zeta(5) \quad (4.17)$$

The integral transform $D \rightarrow R_{e^+e^-}$,

$$\begin{aligned} R_{e^+e^-}(s) &\equiv R(s, \mu^2 = s) = \frac{1}{2\pi i} \int_{-s-i\varepsilon}^{-s+i\varepsilon} \frac{D^{\text{EM}}(\sigma/\mu^2; a_s(\mu^2))}{\sigma} d\sigma \Big|_{\mu^2=s} = \\ &= \left(\sum_i q_i^2 \right) d_R \left(1 + \sum_{m \geq 1} r_m^{\text{NS}} a_s^m(s) \right) + \left(\sum_i q_i \right)^2 \frac{d^{abc} d^{abc}}{d_R} \sum_{n \geq 3} r_n^{\text{S}} a_s^n(s), \end{aligned} \quad (4.18)$$

can be realized as a linear relation by means of the matrix T , $r_j = T^{ji} d_i$, or for the vector representation $R = TD = \sum a_s^j T^{ji} d_i$. The triangular matrix T of the relation can be obtained at any fixed order of perturbative theory [50]. The elements of this matrix below the units on the diagonal contain so-called kinematic “ π^2 -terms” multiplied by the β -function coefficients⁴, see an example of T^{ji} in Appendix C. Taking into account that the β -structure of the normalized coefficients $r_i = r_i^{\text{NS}}/r_1^{\text{NS}}$ is like that for the coefficients d_i , Eqs.(3.1), one can rewrite the results from the matrix in Table 1,

$$r_0 = d_0; \quad r_1^{\text{NS}} = d_1^{\text{NS}}; \quad r_1 = 1; \quad r_2 = d_2; \quad (4.19a)$$

$$r_3[2] = d_3[2] - \frac{\pi^2}{3}; \quad r_3^{\text{S}}[2] = d_3^{\text{S}}[2]; \quad (4.19b)$$

$$r_4[3] = d_4[3] - \pi^2 d_2[1]; \quad r_4[2] = d_4[2] - \pi^2 d_2[0]; \quad r_4[1, 1] = d_4[1, 1] - \frac{5}{6} \pi^2; \quad (4.19c)$$

$$r_5[4] = d_5[4] + \frac{\pi^4}{5} - 2\pi^2 d_3[2]; \quad r_5[0, 2] = d_5[0, 2] - \frac{\pi^2}{2}; \quad r_5[2, 1] = d_5[2, 1] - \pi^2 \left(\frac{7}{3} d_2[1] + d_3[0, 1] \right);$$

$$r_5[1, 0, 1] = d_5[1, 0, 1] - \pi^2; \quad r_5[1, 1] = d_5[1, 1] - \frac{7}{3} \pi^2 d_2[0]; \quad r_5[3] = d_5[3] - 2\pi^2 d_3[1];$$

$$r_5[2] = d_5[2] - 2\pi^2 d_3[0], \quad (4.19d)$$

while the other elements in r_i coincide with ones in d_i ($i \leq 5$). A similar matrix T_{nl}^{S} which relates the coefficients r_n^{S} and d_l^{S} , can be constructed as well. However, in this work we will not consider the π^2 -dependent effects of analytical continuation, which in the singlet case appear first at the $\mathcal{O}(\alpha_s^5)$ -level. Further, we shall use Eqs.(4.19) to construct PT optimized series for R .

⁴ These terms can be obtained for any order of perturbative theory (constrained mainly by the value of RAM) with “Mathematica” routine constructed by V. L. Khandramai and S. V. Mikhailov.

5. BLM AND PMC PROCEDURES AND THE RESULTS

1. General basis

The re-expansion of the running coupling $\bar{a}(t) = a(\Delta, a')$ and its powers in terms of $t - t' = \Delta = \ln(\mu^2/\mu'^2)$ and new coupling a' reads,

$$\begin{aligned}\bar{a}(t) = a(\Delta, a') &= a' - \beta(a') \frac{\Delta}{1!} + \beta(a') \partial_{a'} \beta(a') \frac{\Delta^2}{2!} + \beta(a') \partial_{a'} (\beta(a') \partial_{a'} \beta(a')) \frac{\Delta^3}{3!} + \dots \\ &= \exp(-\Delta \beta(\bar{a}) \partial_{\bar{a}}) \bar{a} |_{\bar{a}=a'},\end{aligned}\quad (5.1)$$

which is the way to write the corresponding RG solution for $a(t)$ through the operator $\exp(-\Delta \beta(a) \partial_a) [\dots] |_{a=a'}$ (see [8] and refs therein). The shift of the logarithmic scale Δ in its turn can be expanded in perturbative series in powers of $a' \beta_0$

$$\begin{aligned}t' &\equiv t - \Delta, \\ \Delta &\equiv \Delta(a') = \Delta_0 + a' \beta_0 \Delta_1 + (a' \beta_0)^2 \Delta_2 + \dots,\end{aligned}\quad (5.2)$$

where the argument of the new coupling a' depends on $t' = t - \Delta$. It is sufficient to take this renormalization scale for the a' argument, which corresponds to the solution on the previous step, rather than to solve the exact equation $a(t - \Delta(a')) = a'$. Re-expansion a in terms of a' leads to rearrangement of the series of perturbative expansion for the RGI quantity D^a (C^{Bjp}), $a^i d_i \rightarrow a'^i d'_i$, where the r.h.s. are expressed in a rather long but evident formulae. In the square brackets below, we write them explicitly:

$$\begin{aligned}a^1 \cdot d_1 &\rightarrow a'^1 \cdot [d'_1 = 1]; \\ a^2 \cdot d_2 &\rightarrow a'^2 \cdot [d'_2 = \beta_0 d_2[1] + d_2[0] - \beta_0 \Delta_0];\end{aligned}\quad (5.3a)$$

$$a^3 \cdot d_3 \rightarrow a'^3 \cdot [d'_3 = \beta_0^2 (d_3[2] - 2d_2[1] \Delta_0 + \Delta_0^2) + \beta_1 (d_3[0, 1] - \Delta_0) + \quad (5.3b)$$

$$\beta_0 (d_3[1] - 2d_2[0] \Delta_0) + d_3[0] - \beta_0^2 \Delta_1]; \quad (5.3c)$$

$$\begin{aligned}a^4 \cdot d_4 &\rightarrow a'^4 \cdot [d'_4 = \beta_0^3 (d_4[3] - 3d_3[2] \Delta_0 + 3d_2[1] \Delta_0^2 - \Delta_0^3 - 2(\Delta_0 - d_2[1]) \Delta_1) + \\ &\quad \beta_1 \beta_0 \left(d_4[1, 1] - (3d_3[0, 1] + 2d_2[1]) \Delta_0 + \frac{5}{2} \Delta_0^2 - \Delta_1 \right) + \\ &\quad \beta_2 (d_4[0, 0, 1] - \Delta_0) + \quad (5.3d)\end{aligned}$$

$$\begin{aligned}&\beta_0^2 (d_4[2] - 3d_3[1] \Delta_0 + 3d_2[0] \Delta_0^2 - 2d_2[0] \Delta_1) + \\ &\beta_1 (d_4[0, 1] - 2d_2[0] \Delta_0) + \quad (5.3e)\end{aligned}$$

$$\beta_0 (d_4[1] - 3d_3[0] \Delta_0) + d_4[0] - \beta_0^3 \Delta_2]; \quad (5.3f)$$

$$\dots \quad \dots \quad a^n \cdot d_n \rightarrow a'^n \cdot [d'_n = \beta_0^{n-1} d_n[n-1] + \dots]. \quad (5.3g)$$

The standard BLM fixes the scale Δ_0 by the requirement $\Delta_0 = d_2[1]$, accumulating 1-loop renormalization of charge just in this new scale [2], at the same time the coefficient $d_2 \rightarrow d_2[0]$ – its “conformal part”. Numerically,

$$\Delta_0 = d_2[1] = \frac{11}{2} - 4\zeta_3 = 0.69177\dots \approx \ln(2) = 0.69314\dots, \quad (5.4)$$

therefore, $Q_{BLM}^2 = \exp(-\Delta_0)Q^2 \approx Q^2/2$.

High order generalization of BLM can be realized in different ways requiring consequently certain equations for the partial shifts $\{\Delta_i\}$. The system of Eqs. (5.3a-5.3g) for d'_i is the basis to construct different BLM generalizations. It is instructive to consider these coefficients $\{d'_i\}$ after the first BLM step; taking $\Delta_0 = d_2[1]$ one obtains

$$d'_2 = d_2[0]; \quad (5.5a)$$

$$d'_3 = \beta_0^2(d_3[2] - d_2[1]^2) + \beta_1(d_3[0, 1] - d_2[1]) + \beta_0(d_3[1] - 2d_2[0]d_2[1]) + d_3[0] - \beta_0^2\Delta_1; \quad (5.5b)$$

$$d'_4 = \beta_0^3(d_4[3] - 3d_3[2]d_2[1] + 2d_2[1]^3) + \beta_2(d_4[0, 0, 1] - d_2[1]) + \beta_1\beta_0(d_4[1, 1] - 3d_3[0, 1]d_2[1] + d_2[1]^2/2 - \Delta_1) + \quad (5.5c)$$

$$\beta_0^2(d_4[2] - 3d_3[1]d_2[1] + 3d_2[0]d_2[1]^2 - 2d_2[0]\Delta_1) + \quad (5.5d)$$

$$\beta_1(d_4[0, 1] - 2d_2[0]d_2[1]) + \quad (5.5e)$$

$$\beta_0(d_4[1] - 3d_3[0]d_2[1]) + d_4[0] - \beta_0^3\Delta_2; \quad (5.5f)$$

$$\dots \quad \dots \quad d'_n = \beta_0^{n-1}d_n[n-1] + \dots \quad (5.5g)$$

The detailed analysis of the d'_i structure was made in [8] in Sec.5. Here we mention a common property of this transform – to obtain the rearrangement of the coefficient at an order $n+1$, $d_{n+1} \rightarrow d'_{n+1}$, one should know its β -structure up to the previous order n . For the partial case of relation $d_{n+1}[n] = (d_2[1])^n$ the β_0^n -terms are canceled (underlined terms) in all the orders even due to the first BLM step. Correspondingly, the special conditions $d_i[0, \dots, 1] = d_2[1]$ will remove the next terms with the leading coefficient β_{i-2} in every order, see double underlined terms in Eqs. (5.5b, 5.5c). The latter conditions were proposed in [5] (see the discussion in Sec.4.2 after Eq. (4.8)), though both of the above hypotheses are far from the results of the direct calculations at $\mathcal{O}(a_s^3)$ in (4.8), really

$$d_3[2] - d_2[1]^2 \approx 3.1035 - 0.4785; \quad d_3[0, 1] - d_2[1] \approx 1.1998 - 0.6918. \quad (5.6)$$

Even more, in QCD the elements $d_{n+1}[n]$ grow as $n!$ due to renormalon contributions [29] and the role of these terms becomes more and more important. To construct the next steps of the PT-optimization with $\Delta_1, \Delta_2, \dots$, one should get more detailed knowledge or provide a hypothesis about the different contributions to d'_n .

2. seBLM and PMC procedures

One of the hypotheses mentioned above is based on the empirical relation between the QCD β -function coefficients β_i , $\beta_i \sim \beta_0^{i+1}$. This can be easily verified for perturbative quenched QCD ($n_f = 0$) numerically and this works in the range of $n_f = 0 \div 5$ of quark flavors for the all known β -coefficients; compare the expressions in Eqs. (A.1, A.2),

$$\beta_i \sim \beta_0^{i+1}, c_i = \beta_i/\beta_0^{i+1} = \mathcal{O}(1). \quad (5.7)$$

This relation allows one to set a hierarchy of contributions in order of the “large value of β_0 ” ($\beta_0 = 11(9)$ at $n_f = 0(3)$) [8]. Of course, relation (5.7) should be broken at some

large enough order of expansion i_0 in virtue of expected Lipatov like asymptotics for the β -function $\beta_i \sim (i!) \beta_0^{i+1}$. Therefore, this hierarchy has a restricted field of application that describes the term “practical approach” in the title of [8].

For this hierarchy the most important terms are of an order of $(\beta_0 a_s)^n / \beta_0$ in order n – underlined below in Eq. (5.8). For illustration we shall use the $R^{\text{NS}}(s)$ -ratio taking into account the result (5.5) for D and relations in Eq. (4.19)

$$r'_2 = d_2[0], \quad (5.8a)$$

$$r'_3 = \beta_0^2 (d_3[2] - d_2[1]^2 - \pi^2/3) + \beta_1 (d_3[0, 1] - d_2[1]) \quad (5.8b)$$

$$+ \beta_0 (d_3[1] - 2d_2[0]d_2[1]) - \beta_0^2 \underline{\Delta_1} + d_3[0]; \quad (5.8c)$$

$$r'_4 = \beta_0^3 (d_4[3] - 3d_3[2]d_2[1] + 2d_2[1]^3 - \pi^2 d_2[1]) + \beta_2 (d_4[0, 0, 1] - d_2[1])$$

$$\beta_1 \beta_0 \left(d_4[1, 1] - 3d_3[0, 1]d_2[1] + d_2[1]^2/2 - 5/6 \pi^2 - \underline{\Delta_1} \right) + \quad (5.8d)$$

$$\beta_0^2 \left(d_4[2] - 3d_3[1]d_2[1] + 3d_2[0]d_2[1]^2 - \pi^2 d_2[0] - 2d_2[0] \underline{\Delta_1} \right) + \quad (5.8e)$$

$$\beta_1 \left(d_4[0, 1] - 2d_2[0]d_2[1] \right) + \quad (5.8f)$$

$$\beta_0 \left(d_4[1] - 3d_3[0]d_2[1] \right) - \beta_0^3 \underline{\Delta_2} + d_4[0]; \quad (5.8g)$$

$$r'_n = \beta_0^{n-1} d_n[n-1] + \dots + \dots \quad (5.8h)$$

The less important terms are suppressed by β_0^{-1} in this order; $(\beta_0 a_s)^n / \beta_0^2$, they are double-underlined in (5.8c, 5.8e, 5.8f), and so on. Following the hierarchy one fixes the values of $\underline{\Delta_1}, \underline{\Delta_2}, \dots$ consequently nullifying at first the most important (1-underlined) β -terms in every order. After that the procedure repeated with the less important terms (double underlined) in all orders, etc. This procedure was called sequential BLM (seBLM) and its result was presented in detail in Sec. 6 of [8] (see Eqs. (6.7, 6.8) there). The discussed hierarchy can also be used for generalization of the NNA approximation, see Appendix C in [50].

The above invented hierarchy ignores a possible difference of values of the elements $d_n[\dots]$ tacitly suggesting that they are of the same order of magnitude. Of course, one can abandon the suggestion of the hierarchy, and to remove *all the β -terms in one mold* consequently order by order. This approach leads to other values of $\underline{\Delta_i} = \bar{\Delta_i}$:

$$\bar{\Delta_0} = d_2[1]; \quad (5.9a)$$

$$\bar{\Delta_1} = \frac{1}{\beta_0^2} \left[\beta_0^2 (d_3[2] - d_2^2[1] - \pi^2/3) + \beta_1 (d_3[0, 1] - d_2[1]) + \beta_0 (d_3[1] - 2d_2[1]d_2[0]) \right] \quad (5.9b)$$

$$\bar{\Delta_2} = \frac{1}{\beta_0^3} \left[\beta_0^3 (d_4[3] - 3d_2[1]d_3[2] + 2(d_2[1])^3 - \pi^2 d_2[1]) + \beta_2 (d_4[0, 0, 1] - d_2[1]) + \right.$$

$$\beta_0 \beta_1 \left(d_4[1, 1] - 3d_3[0, 1]d_2[1] + \frac{3}{2}(d_2[1])^2 - d_3[2] - \pi^2/2 \right) + \beta_1^2 / \beta_0 (d_2[1] - d_3[0, 1]) +$$

$$\left. \beta_1 (\underline{\dots}) + \dots \right], \quad (5.9c)$$

which differ by the underlined “suppressed in the $1/\beta_0$ ” terms from the previous ones in [8]. The complete form for Δ_2 looks cumbersome and it is outlined in Appendix D. The

procedure like this was called PMC later on [3], though for both the cases, seBLM and corrected PMC, the final PT series has the same “conformal terms” $d_n[0]$ as the coefficients of new expansion. The new normalization scale s' follows from Eq. (5.2), taking into account certain expressions for Δ_i in (5.9),

$$R_{e^+e^-}(s) = \left(\sum_i q_i^2 \right) \cdot d_A R^{\text{NS}} + \left(\sum_i q_i \right)^2 \cdot d_A R^{\text{S}}$$

$$R^{\text{NS}}(s) = 1 + 3C_F \{ a(s') + d_2[0] \cdot a^2(s') + d_3[0] \cdot a^3(s') + d_4[0] \cdot a^4(s') + \dots \} \quad (5.10a)$$

$$\ln(s/s') = \bar{\Delta}_0 + a' \beta_0 \bar{\Delta}_1 + (a' \beta_0)^2 \bar{\Delta}_2 + \dots \quad (5.10b)$$

The formulae Eqs.(5.9) and Eqs.(5.10) are the main results of these subsections.

3. Numerical estimates, discussion of PMC/seBLM results

Here we apply the results of the procedure accumulated in Eqs. (5.8,5.9,5.10) for the numerical estimates of the expansion coefficients for a few processes starting with the non-singlet part R^{NS} of the $R_{e^+e^-}(s)$ -ratio. The corresponding singlet part R^{S} can be optimized independently; moreover it is not very important numerically. For the sake of illustration, we put the value $n_f = 3$ for all estimates below. At the very beginning we have the following numerical structure of r_i ,

$$r_2 = \beta_0 \cdot 0.69 + \frac{1}{3} \approx 6.56; \quad (5.11a)$$

$$r_3 = -\beta_0^2 \cdot 0.186 - \beta_1 \cdot 1.2 + \beta_0 \cdot 55.70 - 573.96 \approx -164.5 \quad (5.11b)$$

$$- 15.1 - 76.8 + 501.3 - 573.96$$

$$r_4 \approx -6840.29 \quad (5.11c)$$

At the first BLM setting $\bar{\Delta}_0 \approx 0.69$, $a_s(s) \rightarrow a'_s = a_s(s e^{-0.692} \approx s/2)$ we obtain for the coefficients r'_2, r'_3 — Eqs. (5.12a,5.12b) — the explicit result of the BLM procedure. The value of the second coefficient r'_2 diminishes by an order of magnitude, while r'_3 becomes moderately larger, compare (5.11b) with (5.12b,5.13a),

$$r'_2 = \frac{1}{3}; \quad (5.12a)$$

$$r'_3 = -\beta_0^2 \cdot 0.665 - \beta_1 \cdot 1.892 + \beta_0 \cdot 55.24 - 573.96 \approx -\underline{251.7}; \quad (5.12b)$$

$$- 53.86 - 121.0 + 497.1 - 573.96$$

$$r'_4 \approx -8559.89. \quad (5.12c)$$

At the second step (PMC), we obtain $\bar{\Delta}_1 \approx 3.98$ following Eq.(5.9b) and Eq.(5.2),

$$r''_3 \approx -\underline{573.96}, \quad \bar{\Delta}_1 \approx 3.98, \quad (5.13a)$$

$$r''_4 \approx -11066.1, \quad (5.13b)$$

$$a'_s \rightarrow a''_s = a_s \left(s \cdot e^{-0.692 - 3.98 \beta_0 a'_s(s)} \right), \quad (5.13c)$$

while $r_3'' = d_3[0]$ following the main aim of PMC, see Eq. (5.10a). Due to the strong suppression of the normalization scale by a factor of $\exp[-0.692 - 3.98\beta_0 a'_s(s)]$ the applicability of PT is shifted to the region of very large s ; simultaneously the coefficient r_3'' increases 3 times (cf. (5.11b)). So this procedure makes the convergence of PT worse.

Within the same framework we obtain for the coefficient of the Bjorken function $C_{\text{NS}}^{\text{Bjp}}$

$$c_2 = \beta_0 \cdot 2 - \frac{11}{3} = 14.3(3); \quad (5.14a)$$

$$c_3 = \beta_0^2 \cdot 6.39 + \beta_1 \cdot 0.1084 + \beta_0 \cdot 39.95 - 560.63 \approx 323.44; \quad (5.14b)$$

$$517.5 + 6.9401 + 359.63 - 560.63.$$

$$c_4 \approx 11247.97. \quad (5.14c)$$

At the first BLM step, we do not obtain a significant profit in the first coefficient $c_2 \rightarrow c_2'$, as it was in the previous case of r_2' . But the next order coefficient $c_3 \approx 352.05$ in (5.14b) diminished by two orders (!) of magnitude, $c_3 \rightarrow c_3' \approx 3.444$ at $a_s(Q^2) \rightarrow a'_s = a_s(Q^2 e^{-2} \approx Q^2 \cdot 0.135)$,

$$c_2' = -\frac{11}{3}; \quad (5.15a)$$

$$c_3' = \beta_0^2 \cdot 2.389 - \beta_1 \cdot 1.892 + \beta_0 \cdot 54.63 - 560.63 \approx \underline{3.444}; \quad (5.15b)$$

$$193.5 - 121.06 + 491.63 - 560.63$$

$$c_4' \approx 6361.0. \quad (5.15c)$$

It is interesting that the far fourth coefficient c_4 , (5.14c), reduces twice, $c_4 \rightarrow c_4'$, (5.15c). At the second step (PMC) $\bar{\Delta}_1 \approx 7.32$ and $a'_s \rightarrow a''_s = a_s(Q^2 \cdot \exp[-2 - 7.32\beta_0 a'(Q^2)])$; so the region of applicability of PT is shifted far from the scale of a few GeV^2 . While the value of $|c_3''|$ goes up to the previous order of magnitude, compare (5.15b) with (5.16),

$$c_2'' = -\frac{11}{3}; \quad c_3'' \approx -\underline{560.63}. \quad (5.16)$$

It is instructive to compare this result with one from seBLM (Sec. 5.2), where we remove the first 2 terms in (5.15b) converting them into the normalization scale and holding the last two terms in c_3'' . For this prescription we obtain $\Delta_1 \approx 1.25$,

$$a'_s \rightarrow a''_s = a_s(Q^2 \exp[-2 - 1.25\beta_0 a'(Q^2)]) \quad \text{and} \quad c_3'' \approx -69$$

that looks moderate but is not optimal yet in the sense of series convergence.

Both aforementioned examples demonstrate better convergence at the first BLM step but fail for the optimization of PT at the second PMC step. The reason is the different sign of the terms of r_n (c_n), see the discussion in Sec.6-7 in [8]. It is clear that one should not remove and absorb *all the β -terms* for the PT-optimization but leave a part of them for complete cancellation with the $d_n[0]$ -term. We shall treat the circumstances in this way in the next section.

6. OPTIMIZATION OF THE GENERALIZED BLM PROCEDURE

Indeed, it is not mandatory to absorb all the β -terms as a whole into the new scale Δ_1 (Δ_i) following BLM/PMC, but take instead only those parts of it that are appropriate

for optimization (nullification) of the current order coefficient r_3 (r_{i+2}). At the same time, one should care for the size of the Δ_i – PT coefficients for the shift of scale Δ in (5.2) – not to violate just this expansion.

Let us consider the optimization of R^{NS} at the second BLM step starting with the first step expressions in Eqs.(5.12) and using the general results in (5.8c,5.8e,5.8d). This expression for r_3'' can be rewritten as

$$r_3'' = r_3' - \beta_0^2 \Delta_1 = r_3 - \beta_0^2 d_2[1]^2 - \beta_1 d_2[1] - \beta_0 2d_2[0]d_2[1] - \beta_0^2 \Delta_1. \quad (6.1)$$

The optimization requirement, e.g., $r_3'' = 0$ leads to the expressions for Δ_1 and r_4''

$$r_3'' = 0 \Rightarrow \Delta_1 = r_3'/\beta_0^2 = r_3/\beta_0^2 - d_2[1]^2 - \beta_1/\beta_0^2 d_2[1] - 1/\beta_0 2d_2[0]d_2[1], \quad (6.2a)$$

$$r_4'' = r_4' - r_3' (\beta_1/\beta_0 + 2d_2[0]) . \quad (6.2b)$$

Numerical calculation at $n_f = 4$ gives the estimates for the values of the quantities in Eqs.(6.2),

$$r_3'' = 0, \quad \Delta_1 \approx -3.7, \quad (6.3a)$$

$$r_4'' \approx -4740.52, \quad (6.3b)$$

$$a_s' \rightarrow a_s'' = a_s \left(s \cdot e^{-0.692+3.7\beta_0 a_s'(s)} \right). \quad (6.3c)$$

One may conclude that the PT expansion

$$R^{\text{NS}} = 1 + 3C_F \left\{ a_s'' + \frac{1}{3} \cdot (a_s'')^2 + 0 \cdot (a_s'')^3 + r_4'' \cdot (a_s'')^4 + \dots \right\} \quad (6.4)$$

significantly improves:

(i) $r_3' = 0$, while the value of r_4'' in (6.5e) is less than in (5.11c, 5.12c) and reduces twice in comparison with the PMC estimate in (5.13b) (taken for $n_f = 4$).

(ii) Domain of applicability of the approach extends to a wider region due to the opposite sign at Δ_1 , compare with one for PMC in (5.13a). This makes the NLO “shift” Δ less, which tends numerically to 0 at the boundary of applicability, $\Delta = d_2[1] + \Delta_1 \beta_0 a_s'(s) \approx -0.692 + 3.7\beta_0 a_s'(s)$.

Indeed, following the usual PT condition $|d_2[1]| \gtrsim |\Delta_1 \beta_0 a_s'(s)|$ or $\Delta \lesssim 0$ we get for the boundary $s \gtrsim 10 \text{ GeV}^2$, as it is illustrated in Fig. 1(Left). The factor $\exp[-\Delta]$, entering in the argument of a_s'' in Eq.(6.3c), see solid (red) upper line in Fig. 1(Left), satisfies the conditions $1 \gtrsim \exp[-0.692 + 3.7\beta_0 a_s'(s)] > 1/2$, this factor slowly decreases with s from the value 1. It looks tempting to get and use the exact solution for the coupling a_s^* , following from Eq.(5.2),

$$a_s^*(s) = a_s (s \exp[-\Delta_0 - \Delta_1 \beta_0 a_s^*(s)]),$$

rather than its iteration $a_s''(s)$. It is easy to obtain the useful inequality $a_s'(s) > a_s^*(s) > a_s''(s)$; moreover, the numerical calculation gives that the difference between a_s^* and a_s'' becomes noticeable below $s = 1 \text{ GeV}^2$ for this optimized quantity and for the next one discussed below.

Similar optimization can be performed for $C_{\text{NS}}^{\text{Bjp}}(Q^2)$ ($n_f = 4$). We apply the general combined equations, analogous to the ones of Eqs.(5.3). In these $C_{\text{NS}}^{\text{Bjp}}$ -oriented expressions we fix the conditions $c_2'' = 0$ and $c_3'' = 0$. This leads to the following equations:

$$c_2' = 0, \quad \Delta_0 = c_2/\beta_0 \approx 1.56, \quad (6.5a)$$

$$a_s \rightarrow a_s' = a_s (Q^2 \cdot e^{-1.56}) \quad (6.5b)$$

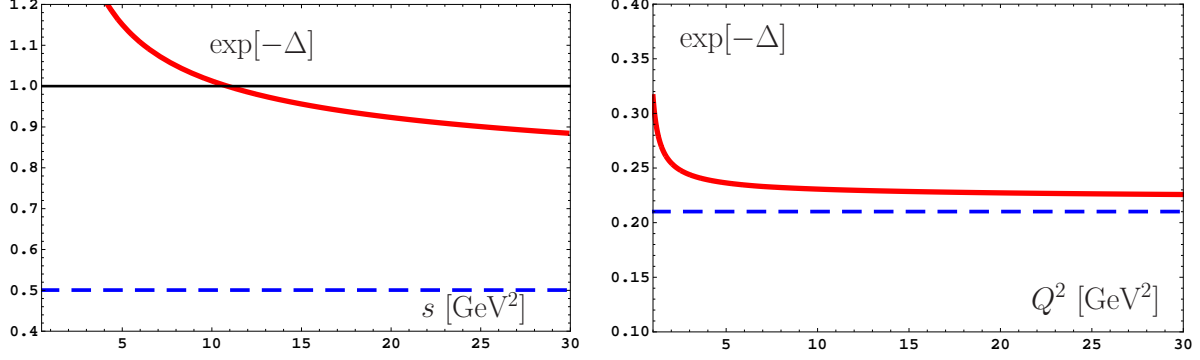


Figure 1: Factors $\exp[-\Delta]$ at coupling scale: (Left) for $R^{\text{NS}}(s)$. Solid (red) upper line – the NLO factor $\exp[-0.692 + 3.7\beta_0 a'_s(s)]$; long dashed (blue) line – the LO BLM one $\exp[-0.692]$. (Right) for $C_{\text{NS}}^{\text{Bjp}}(Q^2)$. Solid (red) upper line – the NLO factor $\exp[-1.56 + 0.396\beta_0 a'_s(Q^2)]$, long dashed (blue) line – the LO $\exp[-1.56]$.

$$c_2'' = c_2' = 0, \quad (6.5c)$$

$$c_3'' = 0, \quad \Delta_1 \approx -0.396, \quad (6.5d)$$

$$c_4'' \approx 4184.64, \quad (6.5e)$$

$$a_s' \rightarrow a_s'' = a_s \left(Q^2 \cdot e^{-1.56 + 0.396\beta_0 a'_s(Q^2)} \right). \quad (6.5f)$$

The new “optimized scale” behaviour of factor $\exp[-\Delta]$ is illustrated in Fig. 1(Right) by solid (red) line, while the broken (blue) line there corresponds to the condition $c_2' = 0$, $\Delta_0 = c_2/\beta_0$ that is not the BLM one. This transformation significantly improves the perturbative series for $C_{\text{NS}}^{\text{Bjp}}$,

$$C_{\text{NS}}^{\text{Bjp}}(Q^2) = 1 - 3C_F \{ a_s'' + 0 \cdot (a_s'')^2 + 0 \cdot (a_s'')^3 + c_4'' \cdot (a_s'')^4 + \dots \} \quad (6.6)$$

in comparison with Eqs.(5.14, 5.15, 5.16). We conclude that for both of the considered quantities the PT series are improved, the corresponding Eqs.(6.3c,6.4) and Eqs.(6.5f,6.6) consist of the main results of this Sec. We did not perform the next step of optimization with the coefficients r_4'' , c_4'' because in this case we lose control under accuracy.

It is clear that Eqs.(6.5,6.4) and Eqs.(6.5,6.6) are not unique optimal solutions because different efficiency functions may be called “optimal”. Therefore, one can satisfy his own efficiency function with the coefficients $\{c_i\}$ basing on the combined Eqs.(5.3) in the plane (Δ_0, Δ_1) or space $(\Delta_0, \Delta_1, \Delta_2, \dots)$ of fitting free parameters Δ_j .

7. CONCLUSION

We have considered the general structure of perturbation expansion of renormalization group invariant quantities in $\overline{\text{MS}}$ -schemes to clarify the effects of charge renormalization and the conformal symmetry breakdown. Following the line started in [8] we arrived at the matrix representation for this expansion, named the $\{\beta\}$ -expansion [9], instead of the standard perturbation series. We discussed in great detail the unambiguity of this representation for Adler D^{NS} -function (or related $R_{e^+e^-}$ -ratio) and for the Bjorken polarized sum rule S^{Bjp} (with the coefficient function $C_{\text{NS}}^{\text{Bjp}}$) for DIS in order $\mathcal{O}(\alpha_s^3)$. The expansion for S^{Bjp} was

obtained by using different parts of the Crewther relation [9] for D^{NS} and the coefficient function $C_{\text{NS}}^{\text{Bjp}}$. Others attempts of this presentation [3–6] were discussed too. We provided new prediction for $C_{\text{NS}}^{\text{Bjp}}(a_s, n_f, n_{\tilde{g}})$ with the MSSM massless gluino $n_{\tilde{g}}$ in order $\mathcal{O}(\alpha_s^3)$ in Eqs.(4.11), Sec.4.2, as a byproduct of our consideration.

Based on the $\{\beta\}$ -expansion we constructed renormalization group transformation for the perturbation series of the considered quantities, Eqs.(5.3) in Sec.5. The initial expansion was split into two parts: A new series for the expansion coefficients, while the other one – for the shift of the normalization scale of the coupling α_s . The contributions from each order can be balanced between these two series. Different procedures of the PT optimization, including PMC [4, 5], and seBLM [8], were discussed and illustrated by numerical estimates. We conclude that the corrected PMC does not provide better PT series convergence and suggest our own scheme of the series optimization in order of $\mathcal{O}(\alpha_s^4)$; the working formulae for R^{NS} of the $R_{e^+e^-}$ -ratio and $C_{\text{NS}}^{\text{Bjp}}$ are presented in Sec.6.

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Appendix A: Explicit formulas for $\beta(n_f, n_{\tilde{g}})$ and $D(n_f, n_{\tilde{g}})$

The required β -function coefficients with the Minimal Supersymmetric Model (MSSM) light gluinos [48] calculated in the $\overline{\text{MS}}$ scheme are,

$$\beta_0(n_f, n_{\tilde{g}}) = \frac{11}{3}C_A - \frac{4}{3}\left(T_R n_f + \frac{n_{\tilde{g}} C_A}{2}\right); \quad (\text{A.1a})$$

$$\beta_1(n_f, n_{\tilde{g}}) = \frac{34}{3}C_A^2 - \frac{20}{3}C_A\left(T_R n_f + \frac{n_{\tilde{g}} C_A}{2}\right) - 4\left(T_R n_f C_F + \frac{n_{\tilde{g}} C_A}{2}C_A\right); \quad (\text{A.1b})$$

$$\begin{aligned} \beta_2(n_f, n_{\tilde{g}}) = & \frac{2857}{54}C_A^3 - n_f T_R \left(\frac{1415}{27}C_A^2 + \frac{205}{9}C_A C_F - 2C_F^2\right) + (n_f T_R)^2 \left(\frac{44}{9}C_F + \frac{158}{27}C_A\right) - \\ & \frac{988}{27}n_{\tilde{g}} C_A (C_A^2) + n_{\tilde{g}} C_A n_f T_R \left(\frac{22}{9}C_A C_F + \frac{224}{27}C_A^2\right) + (n_{\tilde{g}} C_A)^2 \frac{145}{54}C_A. \end{aligned} \quad (\text{A.1c})$$

The β_3 coefficient, which includes the MSSM light gluinos, is not yet known, so we present it here in the standard [52, 53] simplest form

$$\begin{aligned}
\beta_3(n_f) = & C_A^4 \left(\frac{150653}{486} - \frac{44}{9}\zeta_3 \right) + C_A^3 T_R n_f \left(-\frac{39143}{81} + \frac{136}{3}\zeta_3 \right) + C_F^2 T_R^2 n_f^2 \left(\frac{1352}{27} - \frac{704}{9}\zeta_3 \right) \\
& + C_A C_F T_R^2 n_f^2 \left(\frac{17152}{243} + \frac{448}{9}\zeta_3 \right) + C_A C_F^2 T_R n_f \left(-\frac{4204}{27} + \frac{352}{9}\zeta_3 \right) + \frac{424}{243} C_A T_R^3 n_f^3 \\
& + C_A^2 C_F T_R n_f \left(\frac{7073}{243} - \frac{656}{9}\zeta_3 \right) + C_A^2 T_R^2 n_f^2 \left(\frac{7930}{81} + \frac{224}{9}\zeta_3 \right) + \frac{1232}{243} C_F T_R^3 n_f^3 \\
& + 46 C_F^3 T_R n_f + n_f \frac{d_F^{abcd} d_A^{abcd}}{N_A} \left(\frac{512}{9} - \frac{1664}{3}\zeta_3 \right) + n_f^2 \frac{d_F^{abcd} d_F^{abcd}}{N_A} \left(-\frac{704}{9} + \frac{512}{3}\zeta_3 \right) \\
& + \frac{d_A^{abcd} d_A^{abcd}}{N_A} \left(-\frac{80}{9} + \frac{704}{3}\zeta_3 \right). \tag{A.2}
\end{aligned}$$

For the $SU_c(N)$ -group with fundamental fermions the invariants read:

$$T_R = \frac{1}{2}, \quad C_F = \frac{N^2 - 1}{2N}, \quad C_A = N, \quad d^{abc} d^{abc} = \frac{(N^2 - 4)N_A}{N}; \quad N_A = 2C_F C_A \equiv N^2 - 1. \tag{A.3}$$

$$\frac{d_F^{abcd} d_A^{abcd}}{N_A} = \frac{N(N^2 + 6)}{48}, \quad \frac{d_A^{abcd} d_A^{abcd}}{N_A} = \frac{N^2(N^2 + 36)}{24}, \quad \frac{d_F^{abcd} d_F^{abcd}}{N_A} = \frac{N^4 - 6N^2 + 18}{96N^2}. \tag{A.4}$$

The D^{NS} -function evaluated in [25] in the same model in the case when the masses of gluon are neglected⁵ reads

$$D^{\text{NS}}(a_s, n_f, n_{\bar{g}}) = 1 + a_s \cdot (3C_F) \tag{A.5a}$$

$$+ a_s^2 \left\{ -\frac{3}{2} C_F^2 + 2C_F \left[\frac{123}{2} - 44\zeta_3 - (11 - 8\zeta_3)n_{\bar{g}} \right] \frac{C_A}{2} - 2C_F(11 - 8\zeta_3)n_f T_R \right\} \tag{A.5b}$$

$$\begin{aligned}
& + a_s^3 \left\{ -\frac{69}{2} C_F^3 - C_F^2 C_A [127 + 572\zeta_3 - 880\zeta_5 - (36 + 104\zeta_3 - 160\zeta_5)n_{\bar{g}}] \right. \\
& + C_F C_A^2 \left[\frac{90445}{54} - \frac{10948}{9}\zeta_3 - \frac{440}{3}\zeta_5 - \left(\frac{33767}{54} - \frac{4016}{9}\zeta_3 - \frac{80}{3}\zeta_5 \right) n_{\bar{g}} \right. \\
& + \left. \left(\frac{1208}{27} - \frac{304}{9}\zeta_3 \right) n_{\bar{g}}^2 \right] - n_f T_R C_F^2 [29 - 304\zeta_3 + 320\zeta_5] \\
& - n_f T_R C_F C_A \left[\frac{31040}{27} - \frac{7168}{9}\zeta_3 - \frac{160}{3}\zeta_5 - \left(\frac{4832}{27} - \frac{1216}{9}\zeta_3 \right) n_{\bar{g}} \right] \\
& \left. + 3C_F \left[\frac{302}{9} - \frac{76}{3}\zeta_3 \right] \left(\frac{4}{3} T_R n_f \right)^2 \right\} = \tag{A.5c}
\end{aligned}$$

⁵ In the numerical case this expression from [25] coincides with the result of the related numerical calculation of [54].

$$= 1 + a_s(3C_F) + a_s^2(3C_F) \cdot \left\{ \frac{C_A}{3} - \frac{C_F}{2} + \left(\frac{11}{2} - 4\zeta_3 \right) \beta_0(n_f, n_{\bar{g}}) \right\} \quad (\text{A.6a})$$

$$+ a_s^3(3C_F) \cdot \left\{ \left(\frac{302}{9} - \frac{76}{3}\zeta_3 \right) \beta_0^2(n_f, n_{\bar{g}}) + \left(\frac{101}{12} - 8\zeta_3 \right) \beta_1(n_f, n_{\bar{g}}) \right. \\ \left. + \left[C_A \left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5 \right) - C_F(18 + 52\zeta_3 - 80\zeta_5) \right] \beta_0(n_f, n_{\bar{g}}) \right. \\ \left. + \left(\frac{523}{36} - 72\zeta_3 \right) C_A^2 + \frac{71}{3}C_A C_F - \frac{23}{2}C_F^2 \right\} \quad (\text{A.6b})$$

The Bjorken coefficient function $C_{\text{NS}}^{\text{Bjp}}$ of the DIS sum rules calculated first in [38]

$$C_{\text{NS}}^{\text{Bjp}}(a_s, n_f) = 1 + a_s(-3C_F) \quad (\text{A.7a})$$

$$+ a_s^2(-3C_F) \left[-\frac{7}{2}C_F + \frac{23}{3}C_A - \frac{8}{3}T_R n_f \right] \quad (\text{A.7b})$$

$$+ a_s^3(-3C_F) \left\{ \frac{C_F^2}{2} + C_F C_A \left[\frac{176}{9}\zeta_3 - \frac{1241}{27} \right] + C_A^2 \left[\frac{10874}{81} - \frac{440}{9}\zeta_5 \right] \right. \quad (\text{A.7c})$$

$$+ n_f T_R C_F \left[\frac{133}{27} - \frac{80}{9}\zeta_3 \right] - n_f T_R C_A \left[\frac{7070}{81} + 16\zeta_3 - \frac{160}{9}\zeta_5 \right] \\ \left. + \frac{115}{18} \left(\frac{4}{3} n_f T_R \right)^2 \right\}. \quad (\text{A.7d})$$

The prediction for C^{Bjp} obtained in Sec.4.2 of this article under the same conditions as Eq.(A.5) reads

$$C_{\text{NS}}^{\text{Bjp}}(a_s, n_f, n_{\bar{g}}) = 1 + a_s(-3C_F) \quad (\text{A.8a})$$

$$+ a_s^2(-3C_F) \cdot \left\{ \frac{1}{3}C_A - \frac{7}{2}C_F + 2\beta_0(n_f, n_{\bar{g}}) \right\} \quad (\text{A.8b})$$

$$+ a_s^3(-3C_F) \cdot \left\{ \frac{115}{18}\beta_0^2(n_f, n_{\bar{g}}) + \left(\frac{59}{12} - 4\zeta_3 \right) \beta_1(n_f, n_{\bar{g}}) \right. \\ \left. - \left[\left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5 \right) C_A + \left(\frac{166}{9} - \frac{16}{3}\zeta_3 \right) C_F \right] \beta_0(n_f, n_{\bar{g}}) \right. \\ \left. + \left(\frac{523}{36} - 72\zeta_3 \right) C_A^2 + \frac{65}{3}C_F C_A + \frac{C_F^2}{2} \right\}. \quad (\text{A.8c})$$

Appendix B: Natural forms for β -expansion of D^{NS} and C^{NS}

Here we present for completeness the results of (4.8,4.10) in their “natural form” changing only the normalization factors [9], which correspond to the coupling $\frac{\alpha_s}{\pi}$ with

$$\beta_0 = \frac{1}{4} \left(\frac{11}{3}C_A - \frac{4}{3} \left(T_R n_f + n_{\bar{g}} C_A \frac{1}{2} \right) \right), \dots,$$

$$d_1^{\text{NS}} = \frac{3}{4}C_F, \quad (\text{B.1a})$$

$$d_2^{\text{NS}}[1] = \left(\frac{33}{8} - 3\zeta_3\right)C_F, \quad d_2^{\text{NS}}[0] = -\frac{3}{32}C_F^2 + \frac{1}{16}C_FC_A, \quad (\text{B.1b})$$

$$d_3^{\text{NS}}[2] = \left(\frac{151}{6} - 19\zeta_3\right)C_F, \quad d_3^{\text{NS}}[0, 1] = \left(\frac{101}{16} - 6\zeta_3\right)C_F, \quad (\text{B.1c})$$

$$d_3^{\text{NS}}[1] = \left(-\frac{27}{8} - \frac{39}{4}\zeta_3 + 15\zeta_5\right)C_F^2 - \left(\frac{9}{64} - 5\zeta_3 + \frac{5}{2}\zeta_5\right)C_FC_A, \quad (\text{B.1d})$$

$$d_3[0] = -\frac{69}{128}C_F^3 + \frac{71}{64}C_F^2C_A + \left(\frac{523}{768} - \frac{27}{8}\zeta_3\right)C_FC_A^2. \quad (\text{B.1e})$$

$$c_1^{\text{NS}} = -\frac{3}{4}C_F, \quad (\text{B.2a})$$

$$c_2^{\text{NS}}[1] = -\frac{3}{2}C_F, \quad c_2^{\text{NS}}[0] = \frac{21}{32}C_F^2 - \frac{1}{16}C_FC_A, \quad (\text{B.2b})$$

$$c_3^{\text{NS}}[2] = -\frac{115}{24}C_F, \quad c_3^{\text{NS}}[1] = \left(\frac{83}{24} - \zeta_3\right)C_F^2 + \left(\frac{215}{192} - 6\zeta_3 + \frac{5}{2}\zeta_5\right)C_FC_A, \quad (\text{B.2c})$$

$$c_3^{\text{NS}}[0, 1] = \left(-\frac{59}{16} + 3\zeta_3\right)C_F, \quad (\text{B.2d})$$

$$c_3^{\text{NS}}[0] = -\frac{3}{128}C_F^3 - \frac{65}{64}C_F^2C_A - \left(\frac{523}{768} - \frac{27}{8}\zeta_3\right)C_FC_A^2. \quad (\text{B.2e})$$

Appendix C: R-ratio

Table 1 exemplifies the structure of a few first coefficients r_m of the conventional expansion of the R -ratio. Every coefficient r_m contains a number of d_k ($k \leq m$) terms in its expansion, which are shown in the corresponding row. In other words, $r_m = T^{mk}d_k$ (summation in $k = 1, \dots, m$ is assumed), where T^{mk} are the Table entries. Note that the content of this table is limited here only by the restricted place.

Table 1: The table of the T^{mk} -matrix. The one-loop contributions are marked by black, two-loop contributions are marked by red, three-loop contribution — by blue, while the four-loop contribution is colored by green.

	d_1	d_2	d_3	d_4	d_5	d_6
r_1	1					
r_2	0	1				
r_3	$-\frac{(\pi\beta_0)^2}{3}$	0	1			
r_4	0 $-\frac{5\pi^2}{6}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3}3$	0	1		
r_5^a	$\frac{(\pi\beta_0)^4}{5}$ $-\frac{\pi^2}{2}\beta_1^2$ $-\pi^2\beta_0\beta_2$	0 $-\frac{7\pi^2}{3}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3}6$	0	1	
r_6	0 $-\frac{77\pi^4}{60}\beta_0^3\beta_1$ $-\frac{7\pi^2}{6}\beta_1\beta_2$ $-\frac{4\pi^2}{3}\beta_0\beta_3$	$-\frac{(\pi\beta_0)^4}{5}5$ $-\frac{4\pi^2}{3}\beta_1^2$ $-\frac{8\pi^2}{3}\beta_0\beta_2$	0 $-\frac{9\pi^2}{2}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3}10$	0	1

^aThis expression for r_5 was presented first in [51]

Appendix D: Explicit formulae for Δ_i

The explicit expressions for the elements of the proper scales Δ_1 and Δ_2 are given by

$$\Delta_0 = d_2[1]; \quad (D.1)$$

$$\Delta_1 = d_3[2] - d_2^2[1] - \pi^2/3 + \frac{\beta_1}{\beta_0^2} (d_3[0, 1] - d_2[1]) + \frac{1}{\beta_0} \left(\underline{d_3[1] - 2d_2[1]d_2[0]} \right); \quad (D.2)$$

$$\begin{aligned} \Delta_2 = & (d_4[3] - 3d_2[1]d_3[2] + 2(d_2[1])^3 - \pi^2 d_2[1]) + \beta_2/\beta_0^3 (d_4[0, 0, 1] - d_2[1]) + \\ & \beta_1/\beta_0^2 \left[d_4[1, 1] - 3d_3[0, 1]d_2[1] + \frac{3}{2}(d_2[1])^2 - d_3[2] - \pi^2/2 \right] + \beta_1^2/\beta_0^4 (d_2[1] - d_3[0, 1]) + \\ & \beta_1/\beta_0^3 \left(\underline{d_4[0, 1] - d_3[1] - 2d_2[0] (d_3[0, 1] - d_2[1])} \right) + \end{aligned} \quad (D.3)$$

$$1/\beta_0 \left[\underline{d_4[2] - 3d_3[1]d_2[1] + d_2[0] (5d_2[1]^2 - 2d_3[2] - \pi^2/3)} \right] + \quad (D.4)$$

$$1/\beta_0^2 \left[\underline{\underline{d_4[1] - 3d_3[0]d_2[1] + 2d_2[0](2d_2[1]d_2[0] - d_3[1])}} \right]. \quad (D.5)$$

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